Physicists Detect Clue to Material's Unusual Electrical Properties

Karen McNulty Walsh

BNL physicists are studying a mysterious material that may lead to significant advances in the miniaturization of electronics. In the July 27, 2001, issue of *Science* magazine, they offer the first clues explaining the material's newly discovered, unusual electrical properties.

This understanding may result in applications using the material to store electrical charge in high-performance capacitors, and offer insight into how charges behave on the nanoscale—on the order of billionths of a meter.

The material is unusual in that it has an extremely high dielectric constant, a property that determines its ability to become electrically polarized — i.e., separate positive and negative electrical charges. The higher the dielectric constant, the more charge that can be stored, and the smaller the electronic circuits can be made.

In addition, unlike most dielectric materials, this one retains its enormously high dielectric constant over a wide range of temperatures — from 100 to 600 Kelvins (K), or -173 to 327°C — making it ideal for a wide range of applications.

Yet the material's dielectric constant drops precipitously — 1,000-fold — below 100K, with no evidence of structural or phase changes in the atoms.

Therein lies the mystery.

"Such a large change in the electronic properties has implications for the way that charge is distributed within the material," said Christopher Homes, Physics Department. "It's difficult to imagine how those electronic properties can undergo such a large change while the atomic structure remains unaffected."

Previously, scientists at BNL and elsewhere, including Tom Vogt, Stephen Shapiro, and Young-June Kim

Christopher Homes, Tom Vogt, and Stephen Shapiro, Physics Department, who have been studying an unusual dielectric material, are shown at an NSLS infrared beamline. Not present if Young-June Kim, Physics.

of Physics, have looked for hints of changes using x-rays, neutron beams, and other methods—to no avail.

But Homes' technique, measuring optical conductivity, or the material's ability to reflect and absorb varying frequencies of light, revealed a number of unusual changes in the way the atomic structure vibrates.

Homes detected the vibrations by illuminating samples of the substance with varying wavelengths of infrared light at BNL's National Synchrotron Light Source. He measured which wavelengths were reflected and which were absorbed. The absorbed wavelengths are those that match the atoms' natural vibration frequencies.

As the temperature of the substance was cooled below the 100K mark, the absorbed frequencies — and therefore the vibrations — changed.

"Since the vibrations in a solid depend a great deal on how the charges are distributed, the changes in vibrations suggest that the charges can be rearranged without causing a structural distortion," Homes said. "The fact that we see these changes offers the first real glimpse of why this material has such a large dielectric constant, and the mechanism by which it decreases so dramatically below 100K."

The physicists speculate that at temperatures above 100K, pairings of positive and negative electric charges, called dipoles, can flip around quickly, independently of one another.

This property and the high concentration, or density, of dipoles within the solid both contribute to the large dielectric constant, Homes said. If you put the material in an electric field, all the individual dipoles flip into alignment to separate the charges.

But as the material cools, the dipoles "freeze out" in random positions, losing their ability to flip quickly into alignment. This "electronic phase transition" happens in the absence of a structural change.

"Additional research will help us understand this effect and the range of ways this material might be used in microelectronics and other fields," Homes said.

[Editor's note: Reprinted with permission from the BNL Bulletin - August 17, 2001.]